Modeling of mist explosions in the CFD simulator FLACS

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Mist or aerosol explosions represent a potential hazard in the process industries [1]. Gaseous fuel-air explosions are reasonably well understood, and guidance for hazardous area classification for explosive atmospheres resulting from gaseous releases are well established. However, guidance related to flammable mist is scarce, and methods for estimating the consequences of mist explosions often rely on correlations used for gas explosions [2]. In the current version of the computational fluid dynamics (CFD) software FLACS, combustion of oil mists is represented by a method called the butane equivalent fraction. Depending on the molecular weight, concentration and heat of combustion of the fuel, an equivalent butane fraction is calculated to represent the effect of the mist on the flame propagation. Whereas this model can provide reasonable estimates in many situations, there is a need for a more advanced approach.

To this end, the poster describes the implementation of a new model for mist explosions in the CFD simulator FLACS, where the aim is to evaluate the risk, with particular emphasis on quantifying and predicting consequences. The work is based on a model developed previously for liquid releases [3] and on an algebraic slip model [4] for describing droplet-laden flows. It comprised of two parts: a vaporization model and a combustion model.

The study of vaporization and combustion models for droplets can be categorized in three categories: isolated drop, droplet arrays and groups, and sprays. The main differences between these three approaches are the inter-droplet distance and the definition of the gaseous conditions. An isolated droplet is a droplet far enough from other droplets so that the neighboring droplets do not affect the ambient conditions of its gas field. An array encompasses only a few droplets interacting with each other, with the gaseous conditions stated. A group is a big array of droplets, there is no coupling between the gaseous conditions far from the cloud and the droplet calculations. A spray is a group of droplets whom calculations are coupled with the total gas field calculations. The new vaporization model is based on a model by Sirignano [5] called the “robust droplet model”.

Regarding combustion, one of the challenge linked to mist is the existence of three combustion regimes: homogeneous, heterogeneous, and a transition region where both

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homogeneous and heterogeneous take place. The models currently under implementation are based on an approach by Chiu [6] for treating droplet group combustion and another by Sirignano [7] for the mist as a spray. An isolated droplet model was considered. However, with respect to industrial applications this model was deemed irrelevant. The performance of the model system is quantified by simulating different experiments performed previously in Gexcon [8].

References:

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